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Model Based Methodology for Remedial Action Assessment at Hazardous Waste Sites

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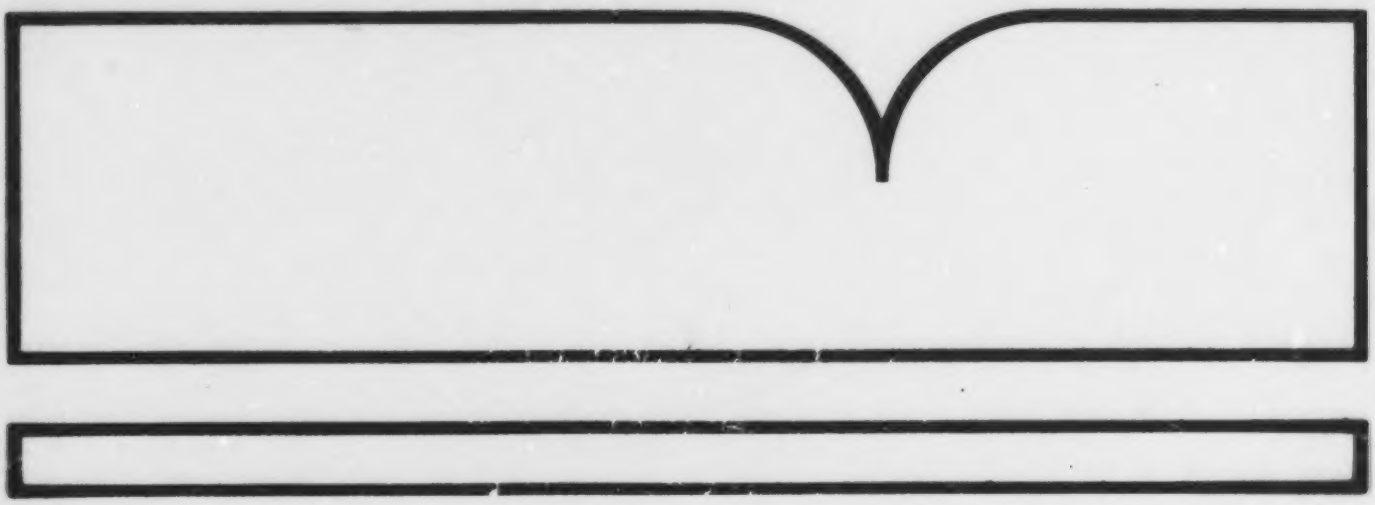

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A MODEL BASED METHODOLOGY FOR REMEDIAL ACTION ASSESSMENT AT HAZARDOUS WASTE SITES

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16. ABSTRACT

The paper describes a remedial action assessment methodology for uncontrolled hazardous waste sites. The model-based methodology consists of three key elements: a set of sophisticated models (one for each hydrologic zone), a data base structure and associated programs to transmit information between models and link the models together, and a set of instructions (referred to as "unit operation modules") for modifying and using the models to simulate the effects of alternative remedial actions. A system of independent, but linked models is developed because such a structure allows 1) use of one or more models independently where modeling of all three zones is not needed and 2) increased user understanding and confidence because each model can be implemented and verified separately. Such a structure requires a model linkage technique which provides transfer of information between models at their boundaries (e.g., the water table boundary between the unsaturated and saturated groundwater zones). Given the diversity of hazardous waste site conditions and potential remedial actions, guidance on the proper application of the model system to remedial action assessment is essential. This is provided through the unit operation modules. The remainder of this paper discusses the approach used to select the specific numerical models, the design of the model system, and the unit operation modules. The paper is for presentation at the Fourth Management of Uncontrolled Hazardous Waste Sites Conference, October 1983, Washington, D. C.

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A MODEL BASED METHODOLOGY FOR REMEDIAL ACTION ASSESSMENT AT HAZARDOUS WASTE SITES

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INTRODUCTION

In the past, selection and design of remedial actions for uncontrolled hazardous waste sites has largely been accomplished through field data collection, simple analyses and engineering judgement. Such approaches are generally satisfactory for most sites. There are a subset of sites, however, where conditions are so complex that simple analyses may not provide enough guidance to allow for the proper selection and design of remedial actions. Given the high economic costs to government and industry associated with site clean-up combined with the future societal cost of inadequate actions, it is important that effective, economical actions be chosen. Thus, there is a need for a remedial action assessment methodology which is flexible enough to provide the appropriate level of analysis and accurate enough to provide confidence in the decisions made.

Recently, several studies involving the evaluation of remedial actions at uncontrolled hazardous waste sites have been successfully accomplished using relatively sophisticated models. Examples are the La Bounty landfill in Charles City, IA[1], Love Canal[2] and a site in Gloucester, Ontario[3]. These studies provide a motivation for the development of a methodology composed of sophisticated models which can address the diverse nature of waste sites. Such a methodology, by expanding on the capabilities demonstrated in these studies, could accurately represent remedial action impacts on the entire hydrologic system (land surface, unsaturated zone and saturated ground water zone).

It is clear from experience to date that two levels of sophistication are needed in hazardous waste site and remedial action assessments: simplified, "desk-top" methods (e.g., nomographs, analytic equations, and hand-held calculator programs) for use where resources such as data, time, money, and user expertise are limited and comprehensive numerical models for use on complex sites that will require costly remedial actions. Consequently, a methodology is being developed that provides: 1) a comprehensive modeling capability by interfacing sophisticated models for the three hydrologic zones, 2) flexibility by incorporating simplified, "desk top" methods which require limited resources in their application and 3) guidance on when to apply each method. This paper focuses on the first issue: the selection and interfacing of sophisticated models.

OVERVIEW OF THE MODEL-BASED METHODOLOGY

The proposed model-based methodology consists of three key elements: a set of sophisticated models (one for each hydrologic zone), a data base structure and associated programs to transmit information between models and link the models together, and a set of instructions (referred to as "unit operation modules") for modifying and using the models to simulate the effects of alternative remedial actions. We have chosen to develop a system of independent, but linked models because such a structure allows 1) use of one or more models independently where modeling of all three zones is not needed and 2) increased user understanding and confidence because each model can be implemented and verified separately. Such a structure requires a model linkage technique which provides transfer of information between models at their boundaries (e.g., the water table boundary between the unsaturated and saturated ground water zones). Given the diversity of hazardous waste site conditions and potential remedial actions, guidance on the proper application of the model system to remedial action assessment is essential. This is provided through the unit operation modules.

The remainder of this paper discusses the approach used to select the specific numerical models, the design of the model system, and the unit operation modules.

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SELECTION OF MODELS FOR REMEDIAL ACTION ASSESSMENT

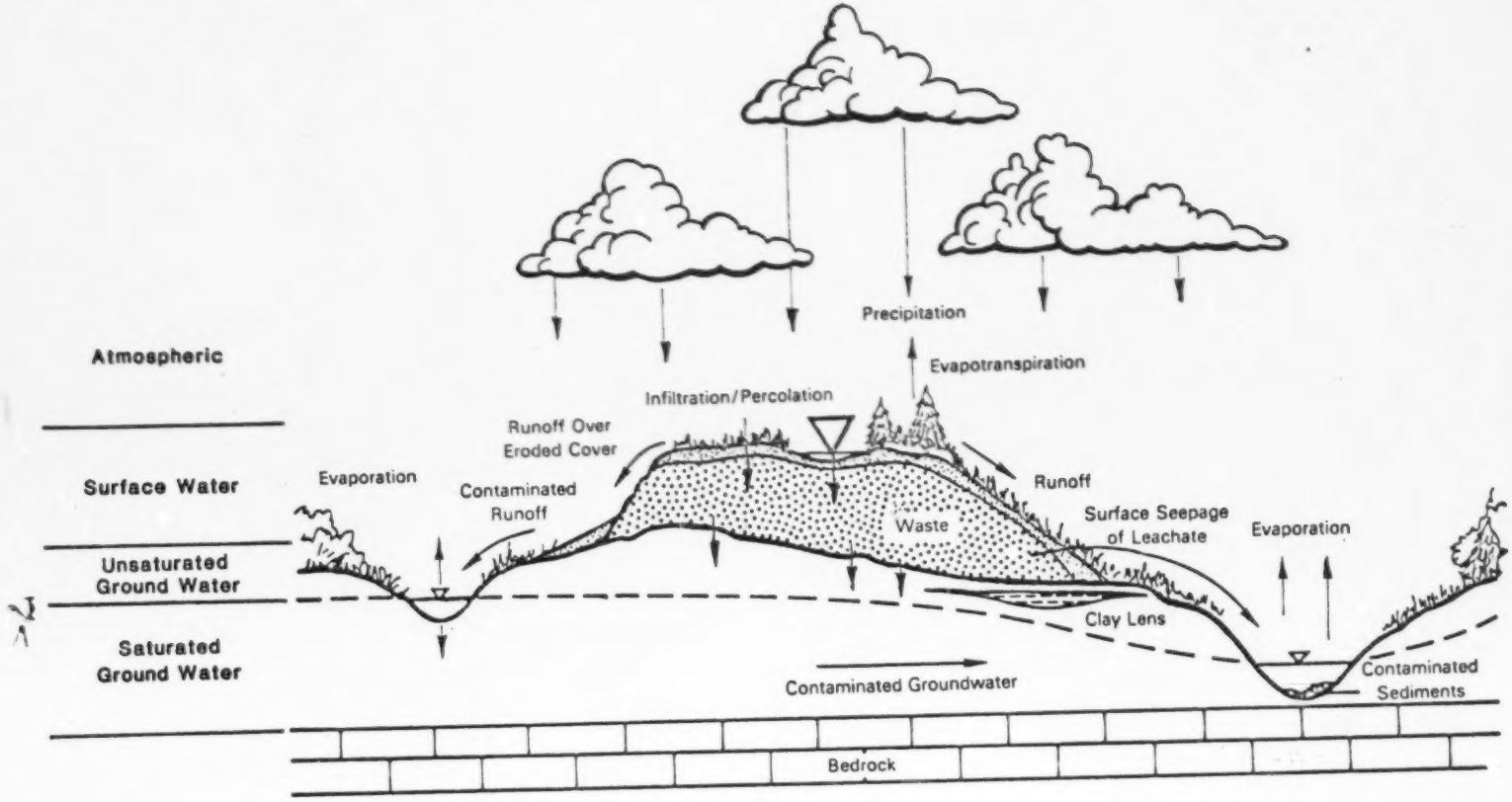
The identification of candidate numerical models for each hydrologic zone was based on the following criteria: model time frame, ability to represent multiple spatial dimensions, representation of key physical and chemical processes, and capacity to represent the changes in geometry and processes caused by specific remedial actions. Final selection of specific models for each of the hydrologic zones was based on the data structure of the model and its compatibility with other selected models, the extent of past model testing and validation, and the quality of available model documentation. These criteria and the selected models will be discussed in this section.

Contaminant transport processes and chemical interactions vary substantially between zones in the hydrologic system. As shown in Figure 1, the hydrologic system can be divided into three zones (surface water, unsaturated ground water, and saturated ground water) plus an atmospheric zone. Key contaminant transport processes within these hydrologic zones include advection, dispersion, sorption, and degradation in all zones. Runoff, evapotranspiration, erosion and infiltration occur in the surface zone. Transport processes between zones include infiltration or seepage from surface to unsaturated zones and leaching from unsaturated to saturated zones. The construction of a waste site in the system alters some of these processes and the installation of remedial actions causes other changes. Inter-zone transfers of water and contaminants may be influenced by pumping or injec-

FIGURE 1

HYDROLOGIC ZONES AND PROCESSES NEAR WASTE DISPOSAL SITES

(AFTER JRB, 1982)



tion wells, interception trenches, or impermeable barriers. Table 1 is a matrix which summarizes the effects of fifteen remedial actions on these key processes.

Model time frame must be dynamic so that variations in the hydrology, process changes over time due to the installation of remedial actions, and the movement of contaminants may be represented. Time step size will vary with the zone and will be shortest in the surface zone where hydrologic changes are rapid. Spatial representation must be a minimum of two dimensions in the saturated zone to represent remedial actions such as impermeable barriers and complex flow conditions. In the unsaturated zone, one dimension may be adequate to represent most actions, but two dimensions will be required to simulate sloping french drains or clay layers with perched water tables. Remedial action representation in the models is also dependent on the ability to model heterogeneous properties such as hydraulic conductivity and adsorption and to vary spatial resolution where abrupt changes in geometry or materials occur. For example, an impermeable barrier requires an abrupt decrease in hydraulic conductivity and an in situ treatment bed requires an abrupt increase in material properties related to adsorption and/or degradation. Table 1 summarizes these changes.

The data structure of a model(i.e., the way information is input, stored, and output by the model) determines the way in which models for the three zones will be linked. If individual model structures are not compatible, linkage of models into an inte-

Table 1 Remedial Actions & Processes Matrix

REMEDIAL ACTIONS	SURFACE ZONE							UNSATURATED ZONE					SATURATED ZONE								SPECIAL CONSIDERATIONS	
	LAND SEGMENT (Single / Multiple)	Adsorption	Degradation	Runoff	Evapo-transpiration	Erosion	INTER-ZONE TRANSFER Infiltration / Seepage	DIMENSION (1,2,3)	Advection	Dispersion	Adsorption	Degradation	INTER-ZONE TRANSFER Leaching	DIMENSION (1,2,3)	Advection	Dispersion	Adsorption	Degradation	INTER-ZONE TRANSFER Pumping / Injection	Volatilization / Methane Release	Heterogeneous Properties	Variable Spatial Resolution
SURFACE CONTROL																						
Grading	S			+		-	-		-				-									
Revegetation	S			-	+	-	+															
Surface Water Diversion and Collection	M			-		-	-		-				-								X	
SUBSURFACE CONTROL																						
Capping & Top Liners				+		-	-	1	-				-								P	
Seepage Basin & Ditches				-			+	2,3	+				+	2	+						P	
Subsurface Drain / Ditches / Bottom Liners								1,2,3					-									X
Impermeable Barriers														2V, 2L,3	+	+					P	X
Ground Water Pumping														2,3	+	+			+			X
Interceptor Trenches														2L	-	-					P	X
WASTE CONTROL																						
Permeable Treatment Bed														1,2			+	+			A	X
Bioreclamation														1				+			D	
Chemical Injection														2,3	+	+	+	+	+		A	X
Solution Mining Extraction							+	1,2	+	+	-	+	+		+	+	-	+	+		A	X
Excavation / Hydraulic Dredging							+	1	-				+		+						P	
GAS MIGRATION CONTROL																				-		

Glossary:

- P = Permeability
- A = Permeability, Adsorption, Degradation & Dispersion
- S = Single Segment
- M = Multiple Segments
- L = Lateral
- V = Vertical

Legend:

- \- = Mitigates Process in Relation to No Action
- \+ = Enhances Process in Relation to No Action

grated system is difficult. Model testing and documentation ensures that selected models operate correctly and can be readily implemented and used efficiently.

Twelve candidate models were selected for evaluation based on the above criteria. A matrix comparing models to evaluation criteria is shown in Table 2. The ability of a given model to represent a specific remedial action can be assessed by comparing the model requirements shown in Table 1 with model capabilities in Table 2. As can be seen, many of the models have similar capabilities, but model validation, case studies, and documentation varies.

One model or model package for each zone was selected based on the above criteria: HSPF (Hydrologic Simulation Program Fortran) for the surface zone, Femwater/Femwaste for the unsaturated zone, and PE3DGW/CHEST for the saturated zone.

- HSPF[5] is a watershed hydrologic model which also simulates erosion, chemical transport in overland flow, streams, and lakes, and infiltration of contaminants. HSPF's multiple land segment and river reach approach allows the representation of heterogeneous land surface and river properties as lumped parameters. A key capability is the model's very flexible data structure and data base management system.
- Femwater/Femwaste[6] is a two-dimensional, vertical plane, finite element model which incorporates both variable time steps and variable spatial resolution. This allows the simulation of complex boundary conditions, abrupt permiabi-

Table 2
Model Review Matrix

MODEL NAME[1] (Reference)	SURFACE ZONE: Land Segment (Single / Multiple)	Infiltration	Evaporation	Runoff	Evapo-transpiration	Erosion	INTER-ZONE TRANSFER: Infiltration / Seepage	Dimension (1,2,3)	Advection	Dispersion	Adsorption	Degradation	INTER-ZONE TRANSFER: Leaching	Dimension (1,2,3)	Advection	Dispersion	Adsorption	Degradation	INTER-ZONE TRANSFER: Pumping / Injection	Volatilization / Vapor Phase	Heterogeneous Properties	Variable Spatial Resolutions	SPECIAL CONSIDERATIONS: Case Studies	Documentation	User's Guide
SURFACE MODEL																									
HSPF (EPA)	(M)	x	x	x	x	x	I						x								x		x	x	x
CREAMS (USDA / Corps of Engrs.)	(S)	x	x	x	x	x	I																x	x	x
MSSWDS (USDA / Corps of Engrs.)	(S)			x	x		I																x	x	x
UNSATURATED ZONE MODEL																									
FEMWATER / FEMWASTE[2] (ORNL)							I/S	2	x	x	x	x	x								x	x	0	x	x
TRUST / MLTRAN (LBL / Battelle)							I/S	2	x		x	x	x								x	x	x	x	0
SEMTRA / FECTRA (Baca)							I	2	x	x	x	x	x								x	x		x	
SATURATED ZONE MODEL																									
FEWA / FEMA (ORNL)													x	2	x	x	x	x	x		x	x		0	x
SWIFT (Intera)													x	3	x	x	x	x	x		x	x	x	x	x
HCTM (Intera)													x	3	x	x	x	x	x		x	x	x		
FE3DGW / CREST (Battelle)													x	3	x	x	x	x	x		x	x	x	x	
AT123D (ORNL)													x	3	x	x	x	x			x	x		x	x
PLASM (Prickett & Lonnquist)													x	7	x	x	x	x	x		x		x	x	x

Footnotes:

1. All models are unsteady state and do not consider volatilization.
2. Flow Model / Transport Model.

Glossary:

(M) = multiple land segment
(S) = single land segment
I = infiltration
S = seepage (handling of seepage pond)

Legend:

x = considered
0 = Case studies - unpublished
Documentation - only for flow model, not for transport code.
User's Guide - only for flow model, not for transport code.

lity changes, and variations in infiltration from the surface over time. It also provides a flexible input and output data structure.

- CFEST[7] is a two- or three-dimensional, finite element model which incorporates variable spatial resolution and allows the simulation of complex boundary conditions and abrupt changes in hydraulic conductivity typical of remedial actions. Wells and drains can be simulated efficiently. In addition, CFEST can simplify data input by performing steps such as grid generation automatically.

DEVELOPMENT OF THE REMEDIAL ACTION MODELING SYSTEM

The modeling system which has been developed relies on communication between the three models to provide simulation of contaminant transport through the three hydrologic zones. Information which must be transferred parallels the movement of the contaminant between zones (refer to Figure 1). Between the surface and unsaturated zones, contaminant and water infiltrates downward from rainfall or surface storage. Leachate reaching the groundwater table moves from the unsaturated zone into the saturated zone. Groundwater and contaminants may reenter the surface zone through recharge to streams and lakes. Remedial actions may also result in transfers. For example, contaminated groundwater can be pumped to the surface, treated and then applied to the land surface (see Table 1). The boundary conditions and source/sink terms in the models must account for these transfers, as shown in Figure 2. Infiltration in HSPF becomes a flux boundary condition

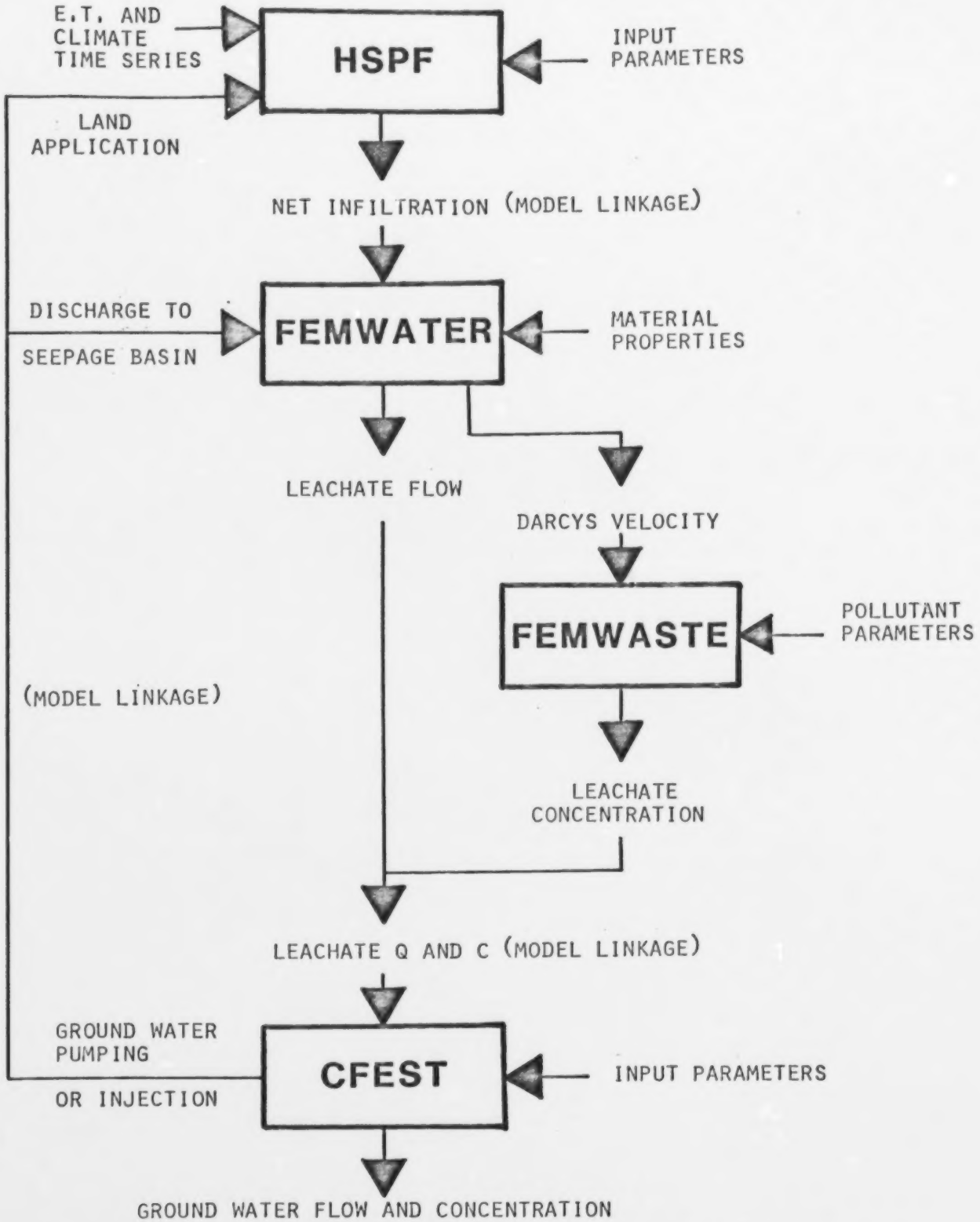


FIGURE 2: SEQUENTIAL EXECUTION OF THE MODEL SYSTEM

in Femwater/Femwaste, while leachate movement through the bottom boundary of Femwater/ Femwaste becomes a flux boundary condition for CFEST. A pumping well is a sink term in appropriate nodes in CFEST and a source term in HSPF if land application is used.

Two approaches to linking the models were considered: 1) a direct coupling of the model equations such that computations in all three zones are performed simultaneously and 2) a "soft linkage" which transfers information sequentially between models. Under soft linkage, the models are run in order (surface, unsaturated, saturated) for all time with no transfer of information against the natural direction of water movement. Any such feedback must be computed in advance and checked subsequently against actual model results. This may involve iterative application of the models. Matching of boundary conditions between models must also be checked to ensure that model results are consistent. For example, soil moisture is computed in different ways in HSPF and Femwater, but must match. The soft linkage approach, as illustrated in Figure 2, was chosen because a direct coupling of the models would be unnecessarily complex and expensive to develop and implement.

Linkage between the three models is implemented through two bridge programs which accept time series data from one model, modify it as needed, and output it to the next model. Data modifications include: 1) temporal aggregation or disaggregation to match model time step requirements, 2) spatial averaging or

interpolation to match boundary value points, 3) unit conversions, and 4) changes in formats required by the programs. Verifying the validity of transferred data is left to the user.

EVALUATION OF REMEDIAL ACTIONS: UNIT OPERATION MODULES

Unit operation modules are a set of descriptive instructions for the simulation of remedial actions using the developed model system. They provide guidance for model parameter and structure adjustment, including: computational element sizes and placement; the use of flux, head and concentration boundary conditions; and process-related parameters such as sorption coefficients, hydraulic conductivities and degradation rates. The modules are written to provide an overview of each remedial action, modeling instructions, a list of affected boundary conditions and model parameters, and typical parameter ranges for the action. Additional information related to the use of the unit modules in conjunction with existing costing procedures, as well as the evaluation of design life and failure mode considerations are also included. Table 1 lists the remedial actions which are currently represented by unit operation modules. These are taken from past studies.[4,8]

Ground water pumping and/or injection are frequently considered remedial actions which have the potential to remove or immobilize contaminant plumes in the saturated zone. Table 3 shows some of the key model-related information which would be included in the unit operation module for ground water pumping. Table 1 provides

TABLE 3: UNIT OPERATION MODULE FOR GROUNDWATER PUMPING
(An Abstract of Module Contents)

Purposes: 1) lower water table to prevent saturation of the waste site, 2) reverse pressure gradient to prevent contaminant movement toward a discharge zone, 3) reduce pressure differences between leaky aquifers to prevent contaminant movement, and 4) create, through pumping/ injection well pairs, a closed flow path which precludes outward contaminant migration and captures the contaminant plume.

Design Variations: 1) pumped water is usually treated before reinjection or surface recharge, 2) off-site disposal of pumpage may be possible, 3) may be used in combination with impermeable barriers and seepage ponds

Affected Zones: saturated zone; unsaturated zone if seepage ponds are used for recharge; surface zone if land application is used

Models Required: CFEST; HSPF if land application is used for recharge; Femwater/ Femwaste if recharged water contains contaminants or seepage ponds are used to recharge treated water

CFEST Modifications: use of a series of sink or source nodes to represent wells; recalculation of heads; adjustment of element boundaries as needed to represent a new water table configuration

Femwater/ Femwaste Modifications: modification of land surface (infiltration) boundary conditions to represent seepage ponds (constant head boundaries); adjustment of bottom element boundaries to represent new water table

HSPF Modifications: creation of land segments and addition of source terms where land application of pumped ground water occurs

Changes in Model Parameters: HSPF - none; Femwater/ Femwaste - increase hydraulic conductivities in elements bounding seepage ponds; CFEST - none

Modeling Issues: discontinuities in head caused by wells and seepage ponds may cause numerical instability unless smaller elements are used in the vicinity of these actions (Femwater and CFEST)

a check list of the important processes and zones affected and indirectly indicates which models must be used to evaluate the action.

CONTINUING DEVELOPMENT EFFORTS

While the modeling system provides a powerful methodology for remedial action assessment, experience with the individual models and with the system is limited. In the coming year, the model system and assessment methodology will be applied to several existing sites presently being evaluated by EPA. Model results will be compared to field observations on the performance of selected actions. Modifications will be made to the modeling system based on the results of the test applications. The methodology will also be used in the site evaluation process. The results of these applications will be used to refine model system application procedures and provide additional guidance for remedial action assessments.

Simplified methods, including hand-held calculator programs, analytical expressions and nomographs, will also be tested, as appropriate, on the existing sites. Comparisons between the performance of the model-based methodology and the simplified methods will be made.

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